The pseudogap regime in the unitary Fermi gas using canonical-ensemble quantum Monte Carlo

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• Introduction

• Thermodynamics of the unitary Fermi gas: experiment and theory

• Canonical-ensemble auxiliary-field Monte Carlo (AFMC) method

• The homogenous unitary Fermi gas: lattice formulation

• Signatures of superfluidity

• Is there a pseudogap regime in the unitary gas?

• Conclusion and outlook
Two-component (spin up/down) fermionic atoms interacting with a short-range interaction $V_0 \delta(r-r')$ characterized by a scattering length $a$.

A crossover from BCS for $(k_F a)^{-1} \sim -\infty$ to BEC for $(k_F a)^{-1} \sim +\infty$.

Of particular interest is the unitary Fermi gas (UFG) describing the limit of strongest interaction $a \to \infty$ or $(k_F a)^{-1} = 0$.

Many interesting properties: universality, scale invariance,…

- A challenging non-perturbative many-body problem
A variety of theoretical methods have been used to study the thermodynamics of the UFG:

**Strong-coupling theories:**

Early theories: Leggett (1980), Nozieres and Schmidt-Rink (1985)

T-matrix approaches

Self-consistent Luttinger-Ward theory

**Quantum Monte Carlo methods:**

Diagrammatic Monte Carlo

Auxiliary-field Monte Carlo (AFMC)

Diffusion Monte Carlo (at T=0)

We use finite-temperature AFMC methods in the canonical ensemble of fixed particle numbers.
Thermodynamics of the UFG

• Superfluid phase transition below a critical temperature $T_c$. However, its nature remains incompletely understood.

• A pseudogap regime above $T_c$ and below $T^*$ was proposed in the UFG, in which pairing correlations exist even though the condensate vanishes.

A pseudogap regime is known from high-$T_c$ superconductors

The pseudogap regime and its extent in the UFG is debated both theoretically and experimentally.

**Pseudogap regime above** $T_c$

Sagi et al, Boulder (PRL 2015): Backbending above $T_c$ in photoemission spectroscopy

**Fermi liquid behavior above** $T_c$

Ku et al, MIT (Science 2012): Equation of state is well described by Fermi liquid theory

Nascimbene et al, Paris (PRL 2011): Spin response compatible with Fermi liquid behavior
Theory

**Pseudogap regime above** $T_c$

Magieriski et al (PRL 2009):
Non-zero gap above $T_c$
(quantum Monte Carlo)

Enss and Haussmann et al (PRL 2009):
No pronounced pseudogap

**Fermi liquid behavior above** $T_c$

Haussmann et al (PRA 2009):

**Spectral weight**

Wlazłowski et al (PRL 2013):
Suppression of spin susceptibility above $T_c$
(quantum Monte Carlo)

Enss and Haussmann (PRL 2012):
No suppression of spin susceptibility
(Luttinger-Ward theory)
Finite-temperature auxiliary-field Monte Carlo (AFMC) method

AFMC is based on the Hubbard-Stratonovich transformation, which describes the Gibbs ensemble $e^{-\beta H}$ at inverse temperature $\beta=1/T$ as a path integral over time-dependent auxiliary fields $\sigma(\tau)$

$$e^{-\beta H} = \int D[\sigma] \ G_\sigma \ U_\sigma$$

$G_\sigma$ is a Gaussian weight and $U_\sigma$ is a propagator of non-interacting particles moving in external auxiliary fields $\sigma(\tau)$

$$\langle \hat{O} \rangle = \frac{\text{Tr} (\hat{O} e^{-\beta \hat{H}})}{\text{Tr} (e^{-\beta \hat{H}}) } = \frac{\int D[\sigma] G_\sigma \langle \hat{O} \rangle_\sigma \text{Tr} \hat{U}_\sigma}{\int D[\sigma] G_\sigma \text{Tr} \hat{U}_\sigma} \quad \text{where} \quad \langle \hat{O} \rangle_\sigma \equiv \frac{\text{Tr}(\hat{O} \hat{U}_\sigma)}{\text{Tr} \hat{U}_\sigma}$$

Grand-canonical quantities in the integrands can be expressed in terms of the single-particle representation matrix $U_\sigma$ of the propagator:

$$\text{Tr} U_\sigma = \det (1 + U_\sigma)$$

The high-dimensional integration over $\sigma$ is evaluated by importance sampling.
**Canonical-ensemble AFMC**

We use exact particle-number projection in the HS transformation

Grand-canonical traces are replaced by canonical traces $Tr \rightarrow Tr_N$

For a finite number $M$ of single-particle states, this can be done by an exact discrete Fourier transform

$$Tr_N U_\sigma = \frac{e^{-\beta \mu N}}{M} \sum_{m=1}^{M} e^{-i\phi_m N} \det(1 + e^{i\phi_m e^{\beta \mu} U_\sigma}) \quad \text{where} \quad \phi_m = 2\pi m / M$$

- The integrand in the HS transformation reduces to matrix algebra in the single-particle space (of typical dimension $\sim 100 - 1000$).

- $O(M^4)$ scaling reduced to $O(M^3)$


Homogenous Fermi gas: a lattice approach

We use a discrete spatial lattice with spacing \( \delta x \) and linear size \( L = N_x \delta x \).

The lattice Hamiltonian for a contact interaction has the form

\[
H = \sum_{k\sigma} \frac{\hbar^2 k^2}{2m} a_{k\sigma}^\dagger a_{k\sigma} + \frac{V_0}{2(\delta x)^3} \sum_{x_i\sigma} \psi_{x_i\sigma}^\dagger \psi_{x_i\sigma}^\dagger \psi_{x_i\sigma} \psi_{x_i\sigma}
\]

where \( k, \sigma \) is a single-particle state with momentum \( k \) and spin \( \sigma \) and \( \psi_{x_i\sigma}^\dagger \) is a creation operator at site \( x_i \) and spin \( \sigma \).

- Our single-particle model space is the complete first Brillouin zone B in \( k \) - a cube with side \( k_c = \pi / \delta x \)

The interaction is normalized to reproduce the two-particle scattering length \( a \) on the lattice:

\[
\frac{1}{V_0} = \frac{m}{4\pi \hbar^2 a} - \frac{mK_3}{4\pi \hbar^2 \delta x} \quad \text{where (for a cube in } k \text{)} \quad K_3 = 2.4427... \quad \text{(Werner, Castin, 2012)}
\]
We carried out AFMC calculation for \(N=20, 40, 80\) and \(130\) atoms on lattices of size \(M=7^3, 9^3, 11^3\) and \(13^3\), respectively, so the filling factor \(\nu = N/M\) remains constant at \(\sim 0.06\).

(i) Condensate fraction \(n\)

Calculated from the largest eigenvalue \(\lambda_{\text{max}}\) of the pair correlation matrix
\[
\langle a_{k_1\sigma_1}^\dagger a_{k_2\sigma_2}^\dagger a_{k_4\sigma_4} a_{k_3\sigma_3} \rangle \quad \text{using} \quad n = \lambda_{\text{max}} / (N/2)
\]

We used finite-size scaling to estimate a critical temperature of \(T_c = 0.130(15) T_F\) at a filling factor of \(\nu \approx 0.06\)
(i) Heat capacity

Numerical differentiation *inside* the path integral using the same fields at $T$ and $T + dT$, and taking into account *correlated* errors: reduces the statistical errors by an order of magnitude [Liu and Alhassid, PRL 87, 022501 (2001)]

First *ab initio* calculation of the heat capacity in AFMC in good agreement with the MIT experiment (lambda point).
(iii) Model-independent pairing gap

We define the energy-staggering pairing gap by

$$\Delta_E = \frac{[2E(N_\uparrow, N_\downarrow - 1) - E(N_\uparrow, N_\downarrow) - E(N_\uparrow - 1, N_\downarrow - 1)]}{2}$$

where $E(N_\uparrow, N_\downarrow)$ is the energy for $N_\uparrow$ spin-up and $N_\downarrow$ spin-down atoms.

First calculation of the energy-staggering pairing gap for the UFG at finite temperature

- Requires the canonical ensemble of fixed particle numbers and uses a reprojection method [Alhassid, Liu and Nakada, PRL 83, 4265 (1999)]
(iv) Static spin susceptibility

\[ \chi_s = \frac{2\beta}{V} \langle (N_\uparrow - N_\downarrow)^2 \rangle \]

Spin-flip excitations require the breaking of pairs
⇒ pairing correlations suppress the spin susceptibility

AFMC, N=40, M=9\(^3\)
N=80, M=11\(^3\)
N=130, M=13\(^3\)
Pantel et al (PRA 2014)
Palestini et al (PRL 2012)
Tajima et al (PRA 2016)
Enss and Haussmann (PRL 2012)
Wlazlowski et al (PRL 2013), M=12\(^3\)
Is there a pseudogap regime in the UFG?

- Pairing gap vanishes above $T_c$

- Moderate suppression of the spin susceptibility above $T_c$

\[ \Rightarrow T^* \leq 0.16 T_F \quad \text{for} \quad \nu \approx 0.06 \]

No clear evidence of pseudogap effects
Two-particle scattering on the lattice

[Werner and Castin (PRA 2012)]

Inverse scattering amplitude (s wave) at relative momentum $k$

$$f_k^{-1} = -ik + k \cot \delta = -ik - \frac{1}{a} + \frac{1}{2} r_e k^2 + ...$$

where $r_e$ is the effective range

On a lattice with spacing $\delta x$: $r_e \approx 0.337 \delta x$

The above expression for $f_k^{-1}$ holds when the complete first Brillouin zone in momentum space is used.

However, when a spherical cutoff of $\pi / \delta x$ is used for the single-particle momentum

$$f_k^{-1} = -ik + \frac{K}{2\pi} - \frac{1}{a} + \frac{1}{2} r_e k^2 + ...$$

where $K$ is the center of mass momentum

A K-dependent shift that does not vanish in the continuum limit $\delta x \rightarrow 0$

- The spherical cutoff does not reproduce the unitary limit
Numerical scattering on the lattice

Low-lying energies of the two-particle system

$k\cot \delta$ vs. $k$

$K = 0$

$K = \frac{2\pi}{L} (1,1,1)$

$N_x = 15$, no cutoff

$N_x = 15$, spherical cutoff

$k\cot \delta$ vs. $k$

$K$ independent

$K$-dependent shift
Thermodynamic observables: no cutoff versus spherical cutoff results

Canonical-ensemble calculations for $N=40$ particles on $M=9^3$ lattice
Conclusion

• We carried out accurate finite-temperature AFMC calculations of the unitary Fermi gas.

• Clear signatures of the superfluid phase transition: heat capacity, condensate fraction, pairing gap, and spin susceptibility

• No clear evidence of a pseudogap regime: pairing gap vanishes and moderate suppression of the spin susceptibility above $T_c$

• Good agreement with experimental data for the condensate fraction, heat capacity, and low-temperature pairing gap

Outlook

• Extrapolate AFMC calculations to zero density (continuum limit) and thermodynamic limit: a major challenge

• More experiments are needed:
  (i) uniform trap
  (ii) spin susceptibility and pairing gap vs. temperature